Combined finite element - particles discretisation for simulation of transport-dispersion in porous media

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1 Introduction

Combining finite element together with particle methods provide one of the best compromise for solving transport problem in porous media. Saturated or non-saturated flows are determined by boundary condition and the media permeability.[4] For real terrain, permeability can consist in various almost constant and imbricated zones with complex shapes. Thus, it is of some interest that the boundary between two adjacent zones coincides with a natural mesh interface and that each element is entirely contains in one such zone. Beside this, solving transport equation by means of particle methods offers two distinctive advantages. The method is unconditionally stable when applied to a pure convective equation, and it does not contain any numerical diffusion if the particle trajectories are correctly computed. Therefore the combination of finite elements and particle method appears to be a straightforward application of the principle : "the right method at the right place".

Although the previous statement provide a consistent basis to build a numerical model, there still remain some options in the choice of the two components themself. To start with, it has long been recognised that the computed flow must satisfied as much as possible the divergence free condition; this can be achieved by selecting a non-conforming or mixed method. Second, there exist many way to design particles methods for the convective part as well as for the dispersion term. For the first one, a so-called streamline method

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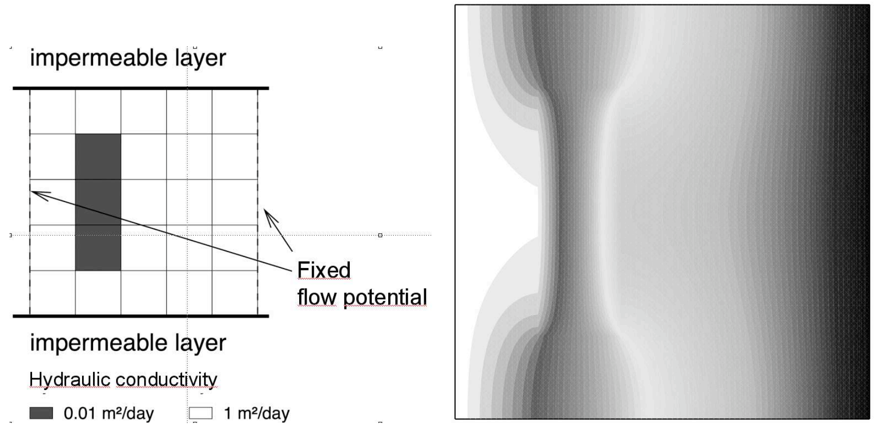

Fig. 1. a) Schematic representation of the domain for the lense test case; b) Flow potential distribution.

can be used as an alternative to the more classical time integration. For the last one, there is a profusion of model including random walk, particle mesh, particle strength exchange and dispersion velocity among others. Our purpose is to compare some of these different strategies in order to provide as clear as possible criteria to be used when designing a solver. Three different points will be successively addressed hereafter : the finite element scheme, the particle trajectories computation and the dispersion simulation.

2 Finite element flow computation

The first point was adressed by considering two finite element schemes to approximate the flow, the usual conforming scheme and a non-conforming scheme (Beaugendre 2006). The latter is quite similar to the more usual mixed hybrid finite element method: it uses one degree of freedom per mesh face and produces a discrete flow field with continuous normal component. The difference with the mixed hybrid finite element approach is that the present scheme can be interpreted as a finite volume box scheme where the mean of governing equations is considered elementwise. Figure 1 shows an example of computed potential flow for the lense test-case.

3 The streamlines method

The trajectories computation was based on the flow computed with the previous finite element method. This is a two steps procedure. First the location of the particle on the finite element mesh have to be determined, second the

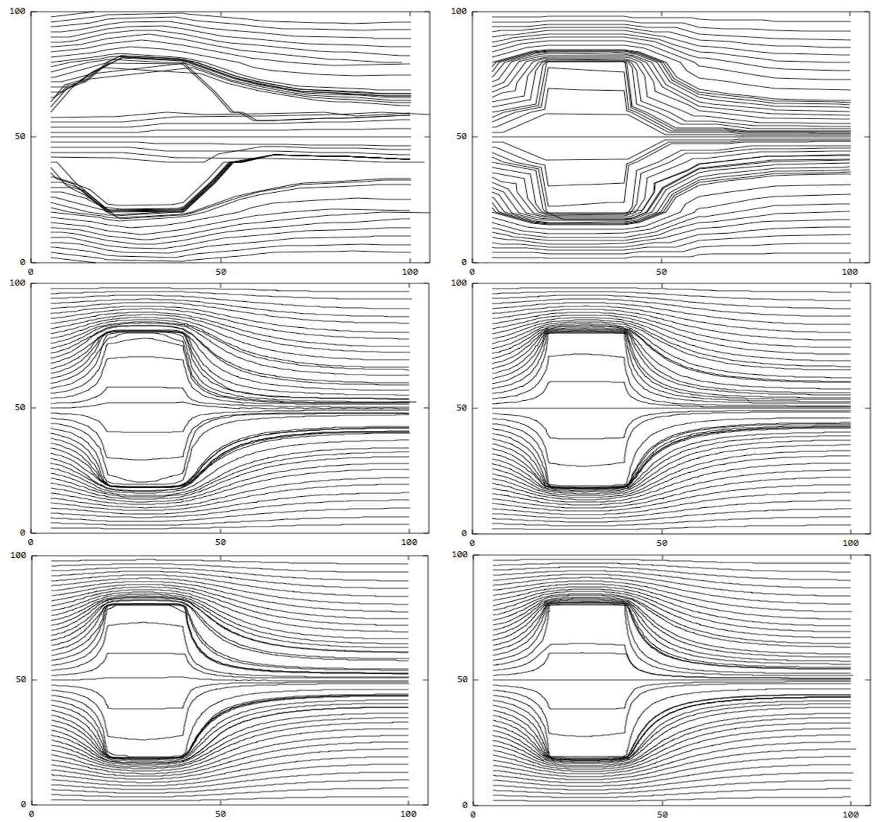

Fig. 2. Comparison of the computed trajectories with non-conservative (left) and conservative (right) flow fields. From top to bottom, finer meshes are used.

trajectories of the particle across the resulting element has to be computed. The first step was achieved by superimposing a regular cartesian grid to the finite element mesh. The cartesian grid cells are selected as small as possible so that a large number of cells cover one single element. Therefore, a particle contains in one grid cell is usually contained by no more than one element. The trajectory computation was performed by using two alternative procedures. The first one consists in a numerical time integration of the differential equation $dX/dt = U$ as usual in particles method. The second consist in using the polynomial form of the velocity field on each element to compute the local streamlines and then the particle trajectory across this element. Associated to this calculation is a time interval corresponding to the particle sojourn within this element also called flight-time. The whole procedure constitutes the streamline method (Matringe 2006).

The resulting method was applied to different test-cases. On figure 2, we present the lense test case streamlines computed from the potential obtained

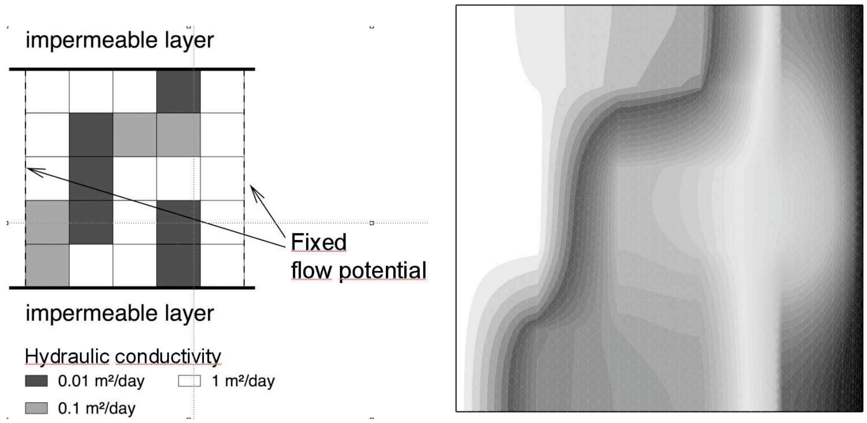

Fig. 3. a) Schematic representation of the domain for the multi-conductivity test case; b) Flow potential distribution.

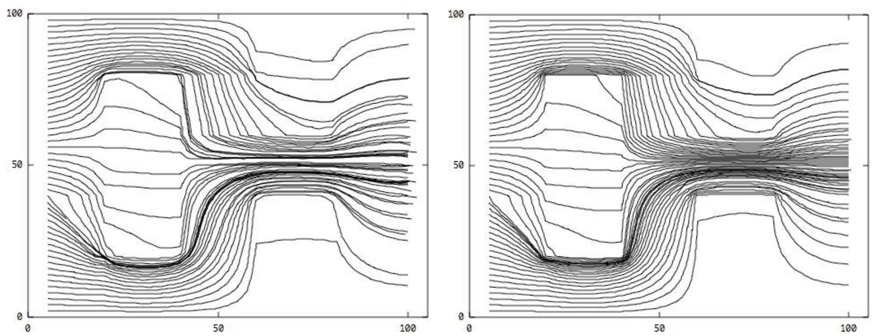

Fig. 4. Computed trajectories for the non-conservative (left) and conservative (right) flow fields.

with the conforming and non conforming method. Three different meshes were used in order to point out the convergence of the two method. It was observed that the non-conforming scheme always provide the best streamlines pattern.

The second test case - figure 4 corresponds to a similar configuration, but uses a fully unstructured mesh. It can be observed from the computed streamlines compared to that of figure 2 that the method still works in this case.

4 Dispersion

The dispersion simulation can be based on many different methods. In the present work, two methods were particularly investigated : the diffusion velocity method and the particle strength exchange (PSE) method. The first

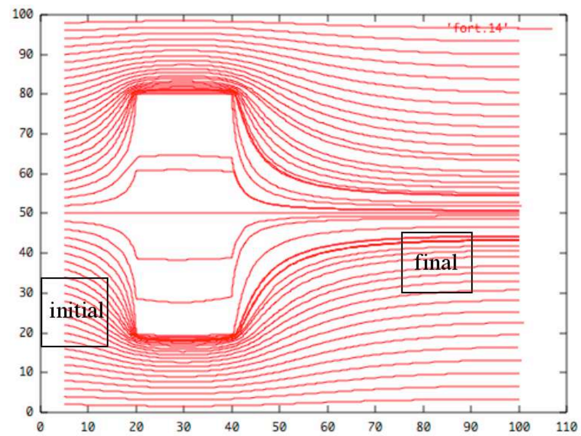

Fig. 5. PSE dispersion. The square indicate the initial and final location of the particle set

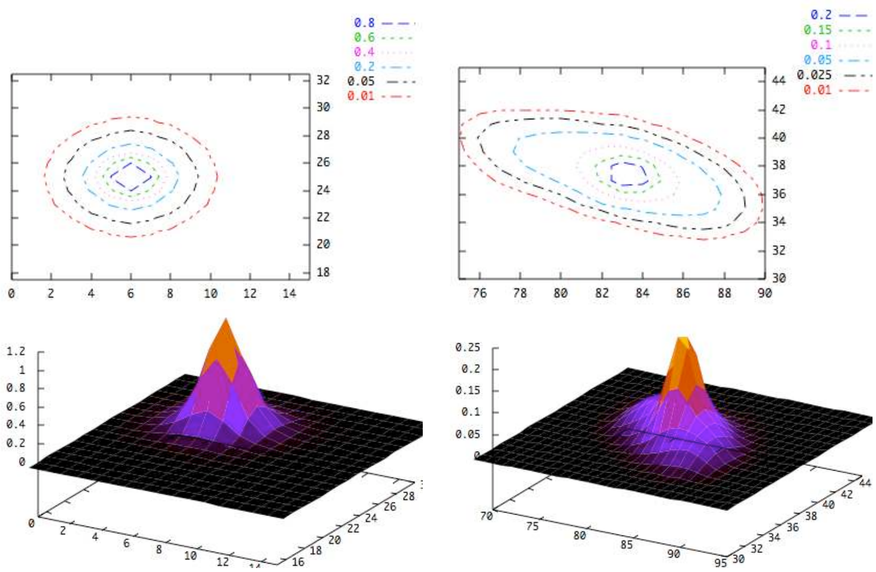

Fig. 6. PSE dispersion : Initial (left) and final(right) concentration

one was selected because it yields modified streamlines, keeping constant the weight associated to each particles weither the second keep the streamlines unchanged and only modifies the particles weight. The first method was assumed to be in agreement with the streamline method concept. It consists in an algebraic manipulation of the original convection-dispersion equation in order to obtain a pure transport equation where the velocity consist in two parts, the original velocity component computed with finite elements and a

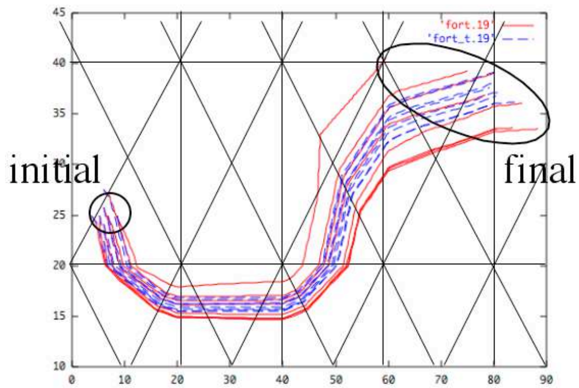

Fig. 7. velocity dispersion : selection of eight particles modified trajectories. dash-lines : original streamlines, continuous lines : modified streamlines

dispersion component which is proportional to the ratio of the gradient by local value of the transported quantity. The method was found to work well in a previous study (Beaudoin 2003) and can be easily combined with any of the two procedures used for the computation of the trajectories. The implementation of the PSE method reduces to the addition of the computation of the particles weight at each time step. It has to be noticed that both method necessitates to have a common time-stepping for all the particle which was not the case when only streamlines were computed.

Eventually, it was found that the PSE metod was the best candidate for extending the streamline method to the case of dispersive flows. The possibility to display initialy the particles along pre-computed streamlines enables to reduce the additional computational work to the particle weights. The application of the velocity diffusion do not permit to keep the same streamlines set for all the computation and, therefore, was found much more CPU-time consuming. It can be obviously guessed that the same drawback definitely plague the application of the Monte-Carlo simulation of dispersion.

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